Shell Effects in Mesoscopic Systems

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A major property of confined Fermi system is the quantisation of single particle motion. It leads to a bunching of levels in the single particle spectrum, known as shells, and gives rise to magic numbers in finite Fermi systems. Consequently, a spherical symmetry leads to very strong shell effects manifested in the stability of the noble gases, nuclei and metallic clusters [1, 2]. Recently the sequence of magic numbers of a two-dimensional harmonic oscillator has been observed in the addition energy for a vertical quantum dot, i.e. in the energy needed to place the extra electron into the dot [3]. In contrast to nuclei and metallic clusters the properties of quantum dots can be controlled by men. The main aim of this talk to discuss the manifestation of shell effects in the mean field approach in different mesoscopic systems, i.e. in nuclei, metallic clusters and quantum dots.

Periodic motion and higher multipoles in nuclei and metallic clusters. When a spherical shell is only partially filled, a breaking of spherical symmetry, resulting in an energy gain, can give rise to a deformed equilibrium shape. Super- and hyperdeformed nuclei are among the most fascinating examples where deviations from the spherical shape are a consequence of strong shell closures giving rise to largest level bunching (largest degeneracy or lowest level density). Nowadays it is recognized that the fine structure in the mass spectra between magic numbers in metallic clusters could be explained via symmetry breaking mechanisms similar to the situation in nuclear physics. It is therefore accepted that cluster deformations can exist, and it is actually confirmed at least for clusters with $A \leq 40$ either by the Clemenger–Nilsson (CN) model (introduced by Nilsson [4] in nuclear physics and applied by Clemenger [5] for clusters) or by a self-consistent Kohn–Sham density–functional method [6] (KS) with deformed jellium backgrounds [7]–[8]. The need for multipole deformations higher than the quadrupole in the mean field approach has been recognized in nuclei and in metallic clusters in numerous calculations to explain experimental data. For instance, the octupole deformed shapes still constitute an intriguing problem of nuclear structure, experimental as well as theoretical (see for review [9]). The hexadecapole deformation is essential for the understanding of equilibrium shapes and the fission process of super- and hyperdeformed nuclei [10]. In the case of metallic clusters, the axial hexadecapole deformation is important for the interpretation of experimental data in simple metals [11]. Inclusion of higher multipoles leads, however, to a nonitegrable problem. In fact, the single particle motion turns out to be chaotic. It is expected that an increasing strength of the

corresponding multipole deformation increases the amount of chaos in the classical potential as quantified by an increasing Lyapunov exponent. Accordingly, in the transition ¿from ordered to chaotic motion the quantum numbers lose their significance, and the system behaves like a viscous fluid [12]. Therefore, a disappearance of shell structure should be expected in the analogous quantum case. However, recently the occurrence of shell structure has been reported for many body systems like nuclei and metallic clusters [13, 14] at strong octupole deformation. A major conclusion of [14] is that, albeit nonintegrable, an octupole admixture to quadrupole oscillator potentials leads, for some values of the octupole strength, to a shell structure similar to a plain but more deformed quadrupole potential. This result shows that there is a tendency of the system to restore the original symmetry (degeneracy of levels) which is destroyed by the octupole term.

The equilibrium deformation is ultimately related to the behavior of the single particle level density of the quantum Hamiltonian. According to the semiclassical theory [15] the frequencies in the level density oscillations of single particle spectra are determined by the corresponding periods of classical closed orbits. The short periodic orbits determine the gross shell structure, whereas contribution of longer orbits give finer details. Analysis of shell structure phenomena in nuclei in terms of classical orbits was started by the work of Balian and Bloch [16] who studied the density of eigenmodes in a spherical cavity with reflecting walls. The importance of deformed shapes for nuclei led to the generalization of this analysis in considering a deformed ellipsoidal well and a deformed harmonic oscillator [1, 17]. Since these problems are integrable, attention was given to regular motion. One of the first attempts to analyze shell structure phenomena and chaotic motion in a quadrupole deformed diffuse cavity was given in [18]. Our approach is based on the connection between shell structure phenomena in the quantum spectrum and ordered motion in the classical analogous case. As it was mentioned above, shell structures in the quantum mechanical spectrum are related to periodic orbits of the corresponding classical problem [1],[16, 17]. The periodic orbits are associated with invariant tori of the Poincaré sections. If the classical problem is chaotic, the invariant tori disintegrate or disappear [25], and the shell structure of the quantum spectrum is affected by the degree of chaos [18]-[24]. The classical treatment is based on the secular perturbation theory [26] and is particularly effective for a two degrees of freedom system. The technique uses action-angle variables of the unperturbed Hamiltonian and averages over the faster phase. Usually, prior to such an operation, a canonical transformation is necessary in order to remove the initial resonance from the unperturbed Hamiltonian (in our case the axial harmonic oscillator without higher multipoles). In the new rotating frame, one of the phases will only measure the slow variation of the variables about the original resonance which now becomes a fixed elliptic point. The problem is then treated by averaging over the remaining faster phase. For super- or hyperdeformed system the frequency of the oscillation in the ϱ-coordinate is twice as fast or faster than that in the z-coordinate. Since the Hamilton function is periodic in both angles, this approximation amounts to keeping the zero order term of its Fourier expansion in the fast moving angle. The integration of the Hamilton function over the angles can be done analytically, which

makes the approximation particularly attractive. The full Hamilton function, being a nonintegrable problem, is approximated by an effective Hamilton function that is obtained by averaging over the fast oscillating angle ϑ_ϱ for the case considered.

An axial harmonic oscillator Hamiltonian (AHO) which is deformed by arbitrary multipoles has the form

$$H = \frac{1}{2m}(p_\varrho^2 + p_z^2 + \frac{p_\phi^2}{\varrho^2}) + \mathcal{U}(r,\vartheta) \tag{1}$$

where

$$\mathcal{U}(r,\vartheta) = \frac{m\omega^2}{2}\left(\varrho^2 + \frac{z^2}{b^2} + r^2(\lambda_3 P_3(\cos\vartheta) + \lambda_4 P_4(\cos\vartheta) + \ldots)\right) \tag{2}$$

with $r^2 = \varrho^2 + z^2$, $\cos\vartheta = z/r$. The z-component of the angular momentum is denoted by p_ϕ and $P_k(\cos\vartheta)$ is the $k-$th order Legendre polynomial. The parameter b characterizes an oblate and a prolate shape for $0 < b < 1$ and $b > 1$, respectively. For a non-vanishing $\lambda_3, \lambda_4, \ldots$ the problem becomes a nonintegrable two degrees of freedom system. Note that the only constant of motion is the total energy. Our interest is focused on the contribution of the octupole and hexadecapole deformation in super- and hyperdeformed system. Therefore, the general potential Eq.(2) is reduced to the form

$$V(\varrho,z) = \frac{m}{2}\omega^2(\varrho^2 + \frac{z^2}{b^2} + \lambda_3\frac{2z^3 - 3z\varrho^2}{\sqrt{\varrho^2+z^2}} + \lambda_4\frac{8z^4 - 24z^2\varrho^2 + 3\varrho^4}{z^2+\varrho^2}). \tag{3}$$

The terms multiplied by λ_3 and λ_4 give rise to octupole and hexadecapole deformations, the respective terms are proportional to $r^2P_3(\cos\vartheta)$ and $r^2P_4(\cos\vartheta)$.

The axial symmetry of the potential given in Eq.(3) guarantees conservation of the z-component of the angular momentum denoted by p_ϕ, the discussion will be focussed on $p_\phi = 0$ unless indicated otherwise. After averaging and rewriting the action variables and the remaining angle ϑ_z in terms of the original momentum and coordinate values we obtain [24]

$$H_{\rm av} = \frac{p_\varrho^2 + p_z^2}{2m} + \frac{m\omega^2}{2}\varrho^2 + U_{\rm eff}(z) \tag{4}$$

where

$$\begin{aligned} U_{\rm eff}(z) = \quad & \frac{m\omega^2}{2}[\frac{z^2}{b^2} + \lambda_3\xi_\varrho^2\frac{\rm sign(z)}{2\pi}(8\frac{z^2}{\xi_\varrho^2}K(-\frac{\xi_\varrho^2}{z^2}) - 3\pi_2{\rm F}_1(\frac{1}{2},\frac{3}{2},2;-\frac{\xi_\varrho^2}{z^2})) + \\ & \lambda_4(\frac{3}{2}\xi_\varrho^2 - 27z^2 + \frac{35|z^3|}{\sqrt{\xi_\varrho^2+z^2}})]. \end{aligned} \tag{5}$$

and $\xi_\varrho^2 = 2J_\varrho/(m\omega) = 2E_\varrho/(m\omega^2)$ which is a constant within the approximation. Here K is the first elliptic integral. Note that the approximated Hamilton function

is separable in the two coordinates with the ϱ-motion being unperturbed. Consequently the frequencies are $\omega_\varrho = \omega$ and $\omega_z = 2\pi/T_z$ with

$$T_z = \sqrt{2m} \int_{z_{\min}}^{z_{\max}} \frac{\mathrm{d}z}{\sqrt{E - E_\varrho - U_{\text{eff}}(z)}} \tag{6}$$

The motion in the z-coordinate is different from the unperturbed motion and its frequency depends on ξ_ϱ, i.e. on the amount of the energy residing in the ϱ-motion. We obtain for the winding number

$$\frac{\omega_\varrho}{\omega_z} = \frac{1}{2}\left(\frac{1}{\sqrt{1/b^2 - 2\lambda_3 + 8\lambda_4}} + \frac{1}{\sqrt{1/b^2 + 2\lambda_3 + 8\lambda_4}}\right). \tag{7}$$

This result is exact for H_{av} when $\xi_\varrho = 0$ (all energy resides in the z-motion), but by the previous argument it applies for large part of phase space. Moreover, it serves as a useful and reliable guideline for the full problem.

The oblate case ($b < 1$) does not lend itself to the same approximation procedure. As was reported in [14] an octupole addition to an oblate quadrupole potential gives no contribution to the zeroth order when averaging over ϑ_z. If only a hexadecapole term is added, the same procedure can be applied and we obtain [22]

$$W_{\text{eff}}(\varrho) = \frac{m}{2}\omega^2\left[\varrho^2 + \lambda_4\left(\frac{35|\varrho^3|}{\sqrt{\varrho^2 + \xi_z^2}} - 32\varrho^2 + 4\xi_z^2\right)\right] \tag{8}$$

with $\xi_z^2 = 2bE_z/(m\omega^2)$. In this case, we find for $\xi_z = 0$, for the winding number

$$\frac{\omega_\varrho}{\omega_z} = b\sqrt{1 + 3\lambda_4}. \tag{9}$$

Note that the admixture of the hexadecapole term to the oblate potential yields, quantum mechanically, an effective plain oblate case but with less deformation. This is in contrast to adding an octupole to a prolate potential where the effective deformation is increased.

The quantum-mechanical results are in line with the classical predictions. We calculated the energy levels of the Hamiltonian

$$H = H_0 + \lambda_3 H_3 + \lambda_4 H_4 \tag{10}$$

where the diagonal matrix H_0 comprises the axial harmonic oscillator, and H_3 and H_4 are the octupole and hexadecapole terms, respectively. The consistent calculation of the matrix elements in a truncated basis is described in [14].

As a quantitative measure for shell structure we use the Strutinsky type analysis (see for details [14, 24]). In accordance with the discussion above, the oblate superdeformed potential produces chaos when the octupole term is switched on. The quantum spectrum has the level statistics ascribed to quantum chaos [20]. The hexadecapole term alone does gives rise to new shell structure; for instance, for $b = 2/5$ and $\lambda_4 \approx 0.1$ oblate superdeformation, i.e. $\omega_\varrho/\omega_z = 1/2$ was established. This is close to the value given by Eq.(9), the difference is explained in [22].

There is remarkable agreement between the manifestation of shell structure for values of the strength parameters λ_3, λ_4, which coincide with the ones predicted by the classical perturbative approach and give rise to stability islands on the Poincaré surfaces of sections. According to the classical approach only even multipoles can decouple the potential of Eq.(1) for an oblate deformation. Therefore, shell structure can be supported for strongly oblate deformed nuclei or clusters only by even multipoles. A further interesting result is the mutual cancellation of the octupole and hexadecapole contribution in the quadrupole deformed system. The classical approach allows to determine the range of parameters of λ_3 and λ_4 where the corresponding quantum mechanical problem of the quadrupole + octupole + hexadecapole potential yields shell structure resembling the plain quadrupole deformation [24]. Along this curve the octupole deformation tends to increase the effective prolate deformation whereas the hexadecapole term produces the opposite effect. In fact, the hexadecapole term can stabilize the octupole deformation in superdeformed systems, since the cancellation curve attains values of λ_3 which are larger than its critical value for $\lambda_4 = 0$. We may speculate that prolate superdeformed nuclei with rather strong octupole deformation could therefore exist. Finally we comment that even though the quantum mechanical treatment shows a certain degree of suppression of classical chaos, the occurrence of a new shell structure which differs from the unperturbed case is clearly brought about by the nonlinear character of the problem.

Filled shells in quantum dots. We choose the harmonic oscillator potential as the effective mean field for the electrons in an isolated quantum dot. While the electron-electron interaction is important for the explanation of certain ground state properties like special values of angular momenta of a quantum dot in a magnetic field [27], a smooth and finite potential which admits bound states can for the lowest few levels always be approximated by the harmonic oscillator potential [28]. This has been confirmed by direct determination of a new effective *oscillator* frequency for two interacting electrons in an external parabolic potential [29] and by calculations of the effective single particle levels within the density-functional theory for electron numbers $N \sim 100$ [30]. For small dot size and small number of electrons the confinement energy becomes prevalent over the Coulomb energy. The experimental identification of the magic numbers of the two-dimensional harmonic oscillator without a magnetic field [3] is the most convincing argument for the validity of this approximation. The effect of an external homogeneous magnetic field can be calculated exactly for a three dimensional (3D) harmonic oscillator potential irrespective of the direction of the field [31]. Our discussion here is based upon the 2D version of the Hamiltonian [31] including spin degree of freedom. The magnetic field acts perpendicular to the plane of motion, i.e. $H = \sum_{j=1}^{A} h_j$ with

$$h = \frac{1}{2m^*}(\vec{p} - \frac{e}{c}\vec{A})^2 + \frac{m^*}{2}(\omega_x^2 x^2 + \omega_y^2 y^2) + \mu^* \sigma_z B. \qquad (11)$$

where $\vec{A} = [\vec{r} \times \vec{B}]/2$, $\vec{B} = (0, 0, B)$ and σ_z is the Pauli matrix. We do not take into account the effect of finite temperature; this is appropriate for experiments which are performed at temperatures $kT \ll \Delta$ with Δ being the mean level spacing. In the following we use meV for the energy and Tesla for the magnetic field strength.

The effective mass which determines the orbital magnetic moment for the electrons is chosen as $m^* = 0.067 m_e$. It leads to $\mu_B^{\rm eff} = 15\mu_B$ while the effective spin magnetic moment is $\mu^* = 0.5\mu_B$.

Shell structure occurs whenever the ratio of the two eigenmodes $\Omega_\pm$ of the Hamiltonian (11) (see Ref.[31]) is a rational number with a small numerator and denominator. If we start with a circular dot ($\omega_x = \omega_y$), the shell structure is particularly pronounced if the ratio is equal to one (for $B = 0$) or two (for $B \approx 1.23$) or three (for $B \approx 2.01$) and lesser pronounced if the ratio is 3/2 (for $B = 0.72$) or 5/2 (for $B = 1.65$). The values given here for B depend on m^* and $\omega_{x,y}$. As a consequence, a material with an even smaller effective mass m^* would show these effects for a correspondingly smaller magnetic field. The magic numbers (including spin) turn out, for $B = 0$, to be the usual sequence of the two dimensional isotropic oscillator, that is $2, 6, 12, 20, \ldots$ [3]. For $B \approx 1.23$ we find a new shell structure *as if* the confining potential would be a deformed harmonic oscillator without magnetic field. The magic numbers are $2, 4, 8, 12, 18, 24, \ldots$ which are just the numbers obtained from the two dimensional oscillator with $\omega_> = 2\omega_<$ ($\omega_>$ and $\omega_<$ denote the larger and smaller value of the two frequencies). Similarly, we get for $B \approx 2.01$ the magic numbers $2, 4, 6, 10, 14, 18, 24, \ldots$ which corresponds to $\omega_> = 3\omega_<$. If we start from the outset with a deformed mean field, i.e. if we choose, say, $\omega_x = (1-\beta)\omega_y$ with $\beta > 0$ two major effects are found: (i) the degeneracies (shell structure) are lifted at $B = 0$ depending on the actual value of β, and (ii) the values for B at which the new shell structures occur are shifted to lower values. The significance of this finding lies in the restoration of shell structures by the magnetic field in an isolated quantum dot that does not give rise to magic numbers at zero field strength due to deformation. We mention that the choice $\beta = 0.5$ would shift the pattern found at $B \approx 1.23$ to the value $B = 0$. It is the shell structure caused by the effective mean field which produces the maxima that are observed experimentally in the addition energy $\mu(A+1) - \mu(A) = E_{A+1} - E_A + e^2/C$ [3]. Here E_A is the single particle energy of the effective mean field in quantum dots, e^2/C is the electrostatic energy and $\mu(A)$ is the chemical potential. The electrostatic energy is much larger than the difference $E_{A+1} - E_A$, however, it is the fluctuations (shell effects) of the difference that matters, at least for small quantum dots. The effect is similar to shell phenomena in nuclear physics and for metallic clusters. The analogy goes further in that, in an isolated small quantum dot, the external magnetic field acts like the rotation on a nucleus thus creating new shell structure; in this way superdeformation (axis ratio 2:1) has been established for rotating nuclei owing to the shell gaps in the single particle spectrum. We now focus on the special cases which give rise to pronounced shell structure, that is when the ratio $\Omega_+/\Omega_- = k = 1, 2, 3, \ldots$, and analyse in detail the circular shape ($\omega_x = \omega_y = \omega_0$). We find for the magnetization

$$M = \mu_B^{\rm eff}(1 - \frac{\omega_L}{\Omega})(\sum\nolimits_- - k\sum\nolimits_+) - \mu^* < S_z > \qquad (12)$$

with $\sum_\pm = \sum_j^A (n_\pm + 1/2)_j$ [31], $\omega_L = \alpha B = \frac{|e|}{2mc} B$ and $\mu_B^{\rm eff} = \hbar\alpha$ being the effective Bohr magneton using the effective mass m^*. The eigenmodes are $\Omega_\pm = (\Omega \pm \omega_L)$ with $\Omega = \sqrt{\omega_0^2 + \omega_L^2}$ [32].

For completely filled shell $< S_z >= 0$, since, for the magnetic field strenghts considered here, the spin orientations cancel each other. ¿From the orbital motion we obtain for the susceptibility

$$\chi = dM/dB = -\frac{{\mu_B^{\rm eff}}^2}{\hbar\Omega}(\frac{\omega_0}{\Omega})^2(\sum\nolimits_+ + \sum\nolimits_-) \tag{13}$$

It follows from Eq.(13) that, for a completely filled shell, the magnetization owing to the orbital motion leads to diamagnetic behaviour. For zero magnetic field ($k = 1$) the system is paramagnetic and the magnetization vanishes ($\sum_- = \sum_+$). The value $k = 2$ is attained at $B \approx 1.23$. When calculating $\sum_-$ and $\sum_+$ we now have to distinguish between the cases, where the shell number N of the last filled shell is even or odd. For the last filled shell number even one finds

$$\sum\nolimits_+ = \frac{1}{12}(N+2)[(N+2)^2+2] \tag{14}$$

$$\sum\nolimits_- = \frac{1}{6}(N+1)(N+2)(N+3) \tag{15}$$

and $M = -\mu_B^{\rm eff}(1-\omega_L/\Omega)(N+2)/2$.

For the last filled shell number odd one finds

$$\sum\nolimits_+ = \frac{1}{2}\sum\nolimits_- = \frac{1}{12}(N+1)(N+2)(N+3) \tag{16}$$

and $M = 0$. Therefore, if $\Omega_+/\Omega_- = 2$, the orbital magnetization vanishes for the magic numbers $4, 12, 24, \ldots$ while it leads to diamagnetism for the magic numbers $2, 8, 18, \ldots$. A similar picture is obtained for $\Omega_+/\Omega- = 3$ which happens at $B \approx 2.01$: for each third filled shell number (magic numbers $6, 18, \ldots$) the magnetization is zero. Since the results presented are due to shell effects, they do not depend on the assumption $\omega_x/\omega_y = 1$ which was made to facilitate the discussion. The crucial point is the relation $\Omega_+/\Omega_- = k = 1, 2, 3, \ldots$ which can be obtained for a variety of combinations of the magnetic field strength and the ratio ω_x/ω_y. Whenever the appropriate combination of field strength and deformation is chosen to yield, say, $k = 2$, our findings apply.

In conclusion: our analysis for nuclei, metallic clusters and quantum dots is based on a rather simple model, and it is true that a realistic single particle spectrum is poorly reproduced by the the harmonic oscillator. However, the lucidity and transparence of the model in describing the phenomena of extreme deformations for nuclei and metallic clusters is superior to any realistic model. The shell structure effects observed for the addition energy of a small isolated quantum dot provide a reliable basis for use the 2D version of the harmonic oscillator Hamiltonian. At certain values of the magnetic field strength shell structures appear in a quantum dot, also in cases where deformation does not give rise to magic numbers at zero field strength. Measurements of the magnetic susceptibility are expected to reflect the properties of the single particle spectrum and should display characteristic patterns depending on the particle number. At certain values of the magnetic field and electron numbers the orbital magnetization vanishes due to shell closure in the quantum dot. This property could be of interest in applications because it enables control of the electron number in small isolated quantum dots.

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